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-> b reg
FILE 'REGISTRY' ENTERED AT 16:36:21 ON 28 NOV 2007
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STRUCTURE FILE UPDATES:   27 NOV 2007  HIGHEST RN 956075-61-9
DICTIONARY FILE UPDATES:  27 NOV 2007  HIGHEST RN 956075-61-9

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TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

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predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=> d que sta l14
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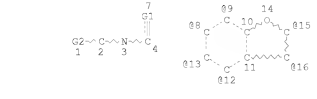


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GRAPH ATTRIBUTES:
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NUMBER OF NODES IS  14

STEREO ATTRIBUTES: NONE
L14         4856 SEA FILE=REGISTRY SSS FUL L12

100.0% PROCESSED  241811 ITERATIONS                      4856 ANSWERS
SEARCH TIME: 00.00.02


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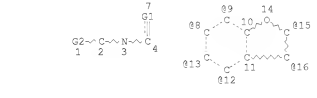


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DEFAULT MLEVEL IS ATOM
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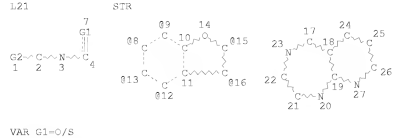

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STEREO ATTRIBUTES: NONE
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SEARCH TIME: 00.00.01

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USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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FILE COVERS 1907 - 28 Nov 2007 VOL 147 ISS 23
FILE LAST UPDATED: 27 Nov 2007 (20071127/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate
substance identification.

=> d bib abs hitstr l27 tot

AN 2007:640830 HCAPLUS
DN 147:72815
TI Preparation of 3-heterocyclylacrylamide derivatives as FabI protein inhibitors for treating bacterial infection
IN Pauls, Henry; Berman, Judd M.
PA Affinium Pharmaceuticals, Inc., Can.
SO PCT Int. Appl., 199pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO2007067416	A2	20070614	2006WO-US45903	20061201
	WO2007067416	A3	20071115		

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RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA

PRAI 2005US-742514P P 20051205
2005US-754024P P 20051223
OS MARPAT 147:72815
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

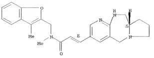
AB The title compds. [I, A = a monocyclic ring of 4-7 atoms containing 0-2 heteroatoms, a bicyclic ring of 8-12 atoms containing 0-4 heteroatoms or a tricyclic ring of 8-12 atoms containing 0-6 heteroatoms wherein the rings are independently aliphatic, aromatic, heteroaryl or heterocyclic in nature, the heteroatoms are selected from N, S or O and the rings are optionally substituted with one or more groups selected from C1-4-alkyl, OR'', cyano, OCF3, F, Cl, Br, iodo; wherein R" = H, alkyl, aralkyl, or heteroaralkyl; R' = H, Me; R = Q-Q12, 6-amino-3-pyridyl; R1 = OH or -O(CH2)nAr; wherein n = an integer from 1 to 6 inclusive; Ar = aryl or heteroaryl; R2 = H or C(O)R3; R3 = H, alkyl, or aryl; R4 = OH or N(R3)2; the two R5 taken together form a spirocycloalkane, a spiroaryl, or a spiroheterocycloalkane; R6 = H, OH, alkyl, or aryl, R7 = alkyl, aryl, cycloalkane, or heterocycloalkane, M = H or OH, or two M taken together form O or N(R3); provided that when R is Q1 or 6-amino-3-pyridyl, R' is (R)-Me] or pharmaceutically acceptable salts thereof are prepared. These compds. including 3-(pyridin-2-yl)acrylamide, 3-(7-oxo-5,6,7,8-tetrahydro[1,8]naphthyridin-3-yl)acrylamide, and 3-(8-oxo-5,7,8,9-tetrahydro-6-oxa-1,9-diazabenzocycloheptan-3-yl)acrylamide derivs. have FabI inhibiting activity, preferably inhabiting the Fab I activity of a microbe with an IC50 of at least 1 order of magnitude lower than the IC50 for inhibiting enoyl CoA hydratase of a mammal. They may also inhibit other enzymes, including those similar to FabI either structurally or functionally, for example, Fab K. Kits and compns. containing the compds. I and methods of treating a subject with a bacterial illness are also disclosed. Thus, 5-bromo-3-(pyridin-2-ylmethoxy)pyridin-2-ylamine was coupled with N-methyl-N-(3-methylbenzofuran-2-ylmethyl)acrylamide in the presence of diisopropylethylamine, Pd(OAc)2, and tris(o-tolyl)phosphine in DMF under refluxing overnight to give 27% (E)-3-[6-amino-5-(pyridin-2-ylmethoxy)pyridin-3-yl]-N-methyl-N-(3-methylbenzofuran-2-ylmethyl)acrylamide. In Staphylococcus aureus FabI enzyme inhibition assays, the invention compds. showed the IC50 values ranging from .apprx.0.05 μM to .apprx.5.0 μM.
IT 941604-33-7P 941604-88-2P, (E)-N-Methyl-N-[(3-

methylbenzofuran-2-yl)methyl]-3-(4-oxo-2,3,4,5-tetrahydro-1H-pyrido[2,3-b][1,4]diazepin-8-yl)acrylamide 941605-02-3P, (R,E)-N-Methyl-N-[1-(3-methylbenzofuran-2-yl)ethyl]-3-(4-oxo-2,3,4,5-tetrahydro-1H-pyrido[2,3-b][1,4]diazepin-8-yl)acrylamide 941605-05-6P, (R,E)-N-[1-(3-Ethylbenzofuran-2-yl)ethyl]-N-methyl-3-(4-oxo-2,3,4,5-tetrahydro-1H-pyrido[2,3-b][1,4]diazepin-8-yl)acrylamide 941605-58-9P, (E)-3-(3,4-Cyclopentyl-2,3,4,5-tetrahydro-1H-pyrido[2,3-e][1,4]diazepin-7-yl)-N-methyl-N-[(3-methylbenzofuran-2-yl)methyl]acrylamide monotrifluoroacetate
RL: PAC (Pharmacological activity), SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of 3-heterocyclylacrylamide derivs. as FabI protein inhibitors for treating bacterial infection)
RN 941604-33-7 HCAPLUS
CN 2-Propenamide, 3-[(9aS)-7,8,9,9a,10,11-hexahydro-5H-pyrido[2,3-e]pyrrolo[1,2-a][1,4]diazepin-3-yl]-N-methyl-N-[(3-methyl-2-benzofuranyl)methyl]-, (2E)-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 941604-32-6
CMF C25 H28 N4 O2

Absolute stereochemistry
Double bond geometry as shown.

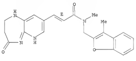


CM 2

CRN 76-05-1
CMF C2 H F3 O2

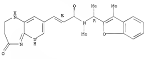
RN 941604-88-2 HCAPLUS
CN 2-Propenamide, N-methyl-N-[(3-methyl-2-benzofuranyl)methyl]-3-(2,3,4,5-tetrahydro-4-oxo-1H-pyrido[2,3-b][1,4]diazepin-8-yl)-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



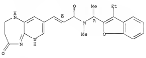
RN 941605-02-3 HCAPLUS
CN 2-Propenamide, N-methyl-N-[(1R)-1-(3-methyl-2-benzofuranyl)ethyl]-3-(2,3,4,5-tetrahydro-4-oxo-1H-pyrido[2,3-b][1,4]diazepin-8-yl)-, (2E)- (CA INDEX NAME)

Absolute stereochemistry
Double bond geometry as shown.



RN 941605-05-6 HCAPLUS
CN 2-Propenamide, N-[(1R)-1-(3-ethyl-2-benzofuranyl)ethyl]-N-methyl-3-(2,3,4,5-tetrahydro-4-oxo-1H-pyrido[2,3-b][1,4]diazepin-8-yl)-, (2E)- (CA INDEX NAME)

Absolute stereochemistry
Double bond geometry as shown.

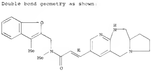


RN 941605-58-9 HCAPLUS
CN 2-Propenamide, 3-(7,8,9,9a,10,11-hexahydro-5H-pyrido[2,3-e]pyrrolo[1,2-a][1,4]diazepin-3-yl)-N-methyl-N-[(3-methyl-2-benzofuranyl)methyl]-, (2E)-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 941605-57-8
CMF C25 H28 N4 O2

Double bond geometry as shown.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

L27 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2007 ACS on STN
AN 2007:454282 HCAPLUS
DN 146:462291
TI Preparation of heterocyclyl acrylamide compounds as FabI inhibitors
IN Manning, David Douglas; Decornez, Helene Yvonne; Surman, Matthew David; Martin, Fernando J. L.; Ramnauth, Jailall; Toro, Andras; Berman, Judd M.; Sampson, Peter; Pauls, Henry; Sargent, Bruce Jeremy
PA Affinium Pharmaceuticals, Inc., Can.
SO Can. Pat. Appl., 232pp.
CODEN: CPXXEB
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	CA 2568914	A1	20051204	2005CA-2568914	20050606
	WO2007053131	A2	20070510	2005WO-US19805	20050606
	WO2007053131	A3	20070802		
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	RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA				
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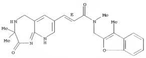
PRAI	2004US-576945P	P	20040604		
	2005WO-US19805	W	20050606		

OS MARPAT 146:462291
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

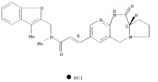
AB Title compds. I [A = monocyclic ring containing 0-2 heteroatoms, bicyclic ring containing 0-4 heteroatoms, tricyclic ring containing heteroatoms containing 0-6 heteroatoms (wherein the rings are independently aliphatic, aromatic, heteroaryl, etc.), the heteroatoms are selected from N, S and O and the rings are optionally substituted with alkyl, CN, OCF3, etc.); R = Q1, etc.; R1 = H, alkyl, aryl, R2 = H, alkyl, aryl, R1 and R2 mey combine to form a fused ring.; R3 = H, alkyl, aryl; R2 and R3 combine to form a spirocyclic ring.; R5 = H, alkyl, aryl] or their pharmaceutically acceptable salts were prepared. For example, Pd(OAc)2 catalyzed coupling reaction of N-(2-ethoxy-3-trifluoromethoxybenzyl)-N-methylacrylamide, e.g., prepared from 2-trifluoromethoxyphenol in 4 steps, with 7-bromo-3,3-dimethyl-1,3,4,5-tetrahydropyrido[2,3-e][1,4]diazepin-2-one followed by treatment with HCl afforded compound II hydrochloride. In E. coli FabI enzyme inhibition assays, the invention compds. showed the IC50 values ranging from 0.05 μM to 100 μM.
IT 709652-79-9P 894851-54-8P 894851-76-4P
894851-82-2P 894851-89-9P 894851-92-4P
894851-97-9P 895237-57-7P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of heterocyclyl acrylamide compds. as FabI inhibitors)
RN 709652-79-9 HCAPLUS
CN 2-Propenamide, N-methyl-N-[(3-methyl-2-benzofuranyl)methyl]-3-(2,3,4,5-tetrahydro-3,3-dimethyl-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, (2E)- (CA INDEX NAME)

L27 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
Double bond geometry as shown.



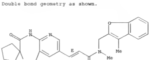
RN 894851-54-8 HCAPLUS
CN 2-Propenamide, 3-[(9aS)-7,8,9,9a,10,11-hexahydro-10-oxo-5H-pyrido[2,3-e]pyrrolo[1,2-a][1,4]diazepin-3-yl]-N-methyl-N-[(3-methyl-2-benzofuranyl)methyl]-, hydrochloride (1:1), (2E)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



RN 894851-76-4 HCAPLUS
CN 2-Propenamide, N-methyl-N-[(3-methyl-2-benzofuranyl)methyl]-3-(1',2',4',5'-tetrahydro-2'-oxospiro[cyclopentane-1,3'-[3H]pyrido[2,3-e][1,4]diazepin]-7'-yl)-, (2E)- (CA INDEX NAME)

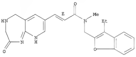
Double bond geometry as shown.



RN 894851-82-2 HCAPLUS
CN 2-Propenamide, N-[(3-ethyl-2-benzofuranyl)methyl]-N-methyl-3-(2,3,4,5-tetrahydro-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.

L27 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



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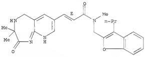
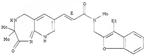
CN 2-Propenamide, N-methyl-N-[(3-propyl-2-benzofuranyl)methyl]-3-(2,3,4,5-tetrahydro-3,3-dimethyl-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



RN 894851-92-4 HCAPLUS
CN 2-Propenamide, N-[(3-ethyl-2-benzofuranyl)methyl]-N-methyl-3-(2,3,4,5-tetrahydro-3,3-dimethyl-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



RN 894851-97-9 HCAPLUS
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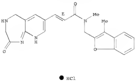
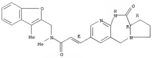
Double bond geometry as shown.



L27 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RN 895237-57-7 HCAPLUS
CN 2-Propenamide, 3-[(9aR)-7,8,9,9a,10,11-hexahydro-10-oxo-5H-pyrido[2,3-e]pyrrolo[1,2-a][1,4]diazepin-3-yl]-N-methyl-N-[(3-methyl-2-benzofuranyl)methyl]-, (2E)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.



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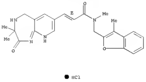
894852-35-8P 894852-90-5P 894853-53-3P
895237-56-6P 895237-67-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of heterocyclyl acrylamide compds. as FabI inhibitors)
RN 709652-77-7 HCAPLUS
CN 2-Propenamide, N-methyl-N-[(3-methyl-2-benzofuranyl)methyl]-3-(2,3,4,5-tetrahydro-3,3-dimethyl-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, hydrochloride (1:1), (2E)- (CA INDEX NAME)

Double bond geometry as shown.



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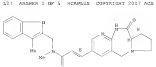
Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.

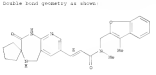
L27 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● HCl

RN 894851-73-1 HCAPLUS
CN 9-Propenamide, N-methyl-N-[(3-methyl-2-benzofuranyl)methyl]-3-(1',2',4',5'-tetrahydro-2'-oxospiro[cyclopentane-1,3'-[3H]pyrido[2,3-e][1,4]diazepin]-7'-yl)-, hydrochloride (1:1). (E)- (CA INDEX NAME)

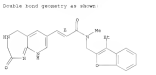
Double bond geometry as shown.



● HCl

RN 894851-80-0 HCAPLUS
CN 1-Propenamide, N-[(3-ethyl-2-benzofuranyl)methyl]-N-methyl-3-(2,3,4,5-tetrahydro-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, hydrochloride (1:1), (2E)- (CA INDEX NAME)

Double bond geometry as shown.



● HCl

RN 894851-84-4 HCAPLUS
CN 2-Propenamide, N-methyl-N-(3-propyl-2-benzofuranyl)methyl]-3-(2,3,4,5-tetrahydro-3,5-dimethyl-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, hydrochloride (1:1), (2E)- (CA INDEX NAME)

Double bond geometry as shown.

L27 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

● HCl

RN 894852-32-6 HCAPLUS
CN 2-Propenamide, N-methyl-N-[(3-methyl-3-benzofuranyl)methyl]-3-(2,3,4,5-tetrahydro-4-methyl-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, hydrochloride (1:1), (2E)- (CA INDEX NAME)

Double bond geometry as shown.

● HCl

RN 894852-38-8 HCAPLUS
CN 2-Propenamide, N-methyl-N-[(3-methyl-3-benzofuranyl)methyl]-3-(2,3,4,5-tetrahydro-4-methyl-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, hydrochloride (1:1), (2E)- (CA INDEX NAME)

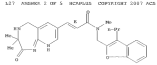
Double bond geometry as shown.

● HCl

RN 894852-40-2 HCAPLUS
CN 2-Propenamide, N-methyl-N-[(3-methyl-1-benzofuranyl)methyl]-3-(2,3,4,5-tetrahydro-2-oxo-4-phenyl-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, hydrochloride (1:1), (2E)- (CA INDEX NAME)

Double bond geometry as shown.

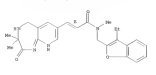
L27 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● HCl

RN 894851-90-2 HCAPLUS
CN 1-Propenamide, N-[(3-ethyl-2-benzofuranyl)methyl]-N-methyl-3-(2,3,4,5-tetrahydro-3,3-dimethyl-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, hydrochloride (1:1). (2E)- (CA INDEX NAME)

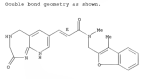
Double bond geometry as shown.



● HCl

RN 894851-95-7 HCAPLUS
CN 2-Propenamide, N-methyl-N-[(3-methyl-3-benzofuranyl)methyl]-3-(2,3,4,5-tetrahydro-3-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



RN 894852-35-9 HCAPLUS
CN 2-Propenamide, N-methyl-N-[(2-methyl-1-benzofuranyl)methyl]-3-(2,3,4,5-tetrahydro-3-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, hydrochloride (1:1), (2E)- (CA INDEX NAME)

Double bond geometry as shown.

L27 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

● HCl

RN 894853-12-3 HCAPLUS
CN 2-Propenamide, N-methyl-N-[(5-methyl-1-benzofuranyl)methyl]-3-[(2S)-2,3,4,5-tetrahydro-2-methyl-3-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl]-, (2E)-, 2,2,2-trifluoroacetate (2:1) (CA INDEX NAME)

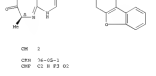
CM 1

CRN 894853-11-2
CMF C23 H24 N4 O3

Absolute stereochemistry.
Double bond geometry as shown.

CM 2

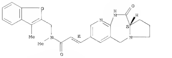
CRN 76-05-1
CMF C2 H F3 O2



RN 894137-86-6 HCAPLUS
CN 2-Propenamide, 3-[(5aR)-7,8,9,9a,10,11-hexahydro-10-oxo-5H-pyrido[2,3-e]pyrrolo[1,2-a][1,4]diazepin-3-yl]-N-methyl-N-[(3-methyl-2-benzofuranyl)methyl]-, (2E)- (CA INDEX NAME)

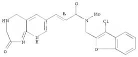
Absolute stereochemistry. Rotation (+)
Double bond geometry as shown.

L27 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 895237-67-9 HCAPLUS
CN 2-Propenamide, N-[(3-chloro-2-benzofuranyl)methyl]-N-methyl-3-(2,3,4,5-tetrahydro-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



L27 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2007 ACS on STN
AN 2006:636869 HCAPLUS
DN 145:103734
TI Compositions comprising multiple antibiotic agents including a FabI inhibitor, methods of using the same, and preparation of the heterocycle FabI inhibitors
IN Berman, Judd M.; Schmid, Molly B.; Mendlein, John D.; Kaplan, Nachum
PA Affinium Pharmaceuticals, Inc., Can.
SO U.S. Pat. Appl. Publ., 192 pp., which which
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US2006142265	A1	20060629	2005US-0231298	20050919
	WO2004082586	A2	20040930	2004WO-IB01261	20040317
	WO2004082586	A3	20041223		

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RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRAI	2003US-455189P	P	20030317
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	2003US-488379P	P	20030718
	2004WO-IB01261	A2	20040317

OS MARPAT 145:103734
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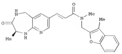
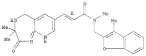


II

AB The invention is directed to antibacterial compns. comprising an NADH (or NADPH)-dependent enoyl-acyl carrier protein (ACP) reductase (FabI, previously designated EnvM) inhibitor of formula (Y1)a-A-CH(R1)-NR1CO-L-R2 (I) and at least one other antibiotic/antibacterial agent [L = alkyl, alkenyl, or cycloalkyl which may be substituted by one or more R1; A = (un)substituted bicyclic heteroaryl of 8-12 atoms or a tricyclic ring of 12-16 atoms, containing 1-4 heteroatoms selected from N, S, and O; R1 = H, cyclo/alkyl, alk/aryl; R2 = heterocyclyl; a = 0-4, Y1 = -(CH2)n-CO-NR4R5; R4 = water solubilizing group; R5 = H, cyclo/alkyl; n = 0-4[. The antibacterial composition exhibits a synergistic antibacterial effect compared to its individual components. Thus, bromination of (S)-2-methyl-1,2,4,5-tetrahydropyrido[2,3-e][1,4]diazepin-3-one (preparation given), coupling of the bromide with N-methyl-N-[(3-methylbenzofuran-2-yl)methyl[acrylamide, and acidulation of the free base (no data) with TFA gave pyridodiazepine II•TFA. Selected I inhibited FabI with a Ki < 1 nM, an MIC (minimal inhibitory concentration) < 0.125 μg/mL, and an IC50 < 10 nM.
IT 709652-79-9P, (E)-3-(3,3-Dimethyl-2-oxo-2,3,4,5-tetrahydro-1H-pyrido[2,3-e][1,4]diazepin-7-yl)-N-methyl-N-[(3-methylbenzofuran-2-yl)methyl]-2-propenamide
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic

L27 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(bactericide; compns. comprising multiple antibiotic agents and prepn. of heterocycle FabI inhibitor)
RN 709652-79-9 HCAPLUS
CN 2-Propenamide, N-methyl-N-[(3-methyl-2-benzofuranyl)methyl]-3-(2,3,4,5-tetrahydro-3,3-dimethyl-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, (2E)- (CA INDEX NAME)

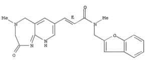
Double bond geometry as shown.



IT 709651-33-2P, (E)-N-[(Benzofuran-2-yl)methyl]-N-methyl-3-(4-methyl-2-oxo-2,3,4,5-tetrahydro-1H-pyrido[2,3-e][1,4]diazepin-7-yl)-2-propenamide monohydrochloride 709651-48-9P, (E)-N-Methyl-N-(3-methylbenzofuran-2-ylmethyl)-3-(4-methyl-2-oxo-2,3,4,5-tetrahydro-1H-pyrido[2,3-e][1,4]diazepin-7-yl)-2-propenamide monohydrochloride 709651-53-6P, (E)-N-Methyl-N-(2-methylbenzofuran-3-ylmethyl)-3-(4-methyl-2-oxo-2,3,4,5-tetrahydro-1H-pyrido[2,3-e][1,4]diazepin-7-yl)-2-propenamide monohydrochloride 709651-82-1P, (E)-N-Methyl-N-(3-methylbenzofuran-2-ylmethyl)-3-[4-[3-(morpholin-4-yl)propyl]-2-oxo-2,3,4,5-tetrahydro-1H-pyrido[2,3-e][1,4]diazepin-7-yl]-2-propenamide monohydrochloride 709651-85-4P, (E)-N-Methyl-N-(2-methylbenzofuran-3-ylmethyl)-3-[4-[3-(morpholin-4-yl)propyl]-2-oxo-2,3,4,5-tetrahydro-1H-pyrido[2,3-e][1,4]diazepin-7-yl]-2-propenamide monohydrochloride 709652-77-7P 894851-54-8P 894851-55-9P 894851-73-1P 894851-80-0P, (E)-N-[(3-Ethylbenzofuran-2-yl)methyl]-N-methyl-3-(2-oxo-2,3,4,5-tetrahydro-1H-pyrido[2,3-e][1,4]diazepin-7-yl)-2-propenamide hydrochloride 894851-84-4P 894851-90-2P 894851-97-9P, (E)-N-Methyl-N-[(3-methylbenzofuran-2-yl)methyl]-3-(2-oxo-2,3,4,5-tetrahydro-1H-pyrido[2,3-e][1,4]diazepin-7-yl)-2-propenamide hydrochloride 894852-25-6P, (E)-N-Methyl-N-[(3-methylbenzofuran-2-yl)methyl]-3-(3-oxo-2,3,4,5-tetrahydro-1H-pyrido[2,3-e][1,4]diazepin-7-yl)-2-propenamide hydrochloride 894852-32-5P, (E)-N-Methyl-N-[(2-methylbenzofuran-3-yl)methyl]-3-(4-methyl-3-oxo-2,3,4,5-tetrahydro-1H-pyrido[2,3-e][1,4]diazepin-7-yl)-2-propenamide hydrochloride 894852-35-8P, (E)-N-Methyl-N-[(3-methylbenzofuran-2-yl)methyl]-3-(4-methyl-3-oxo-2,3,4,5-tetrahydro-1H-pyrido[2,3-e][1,4]diazepin-7-yl)-2-propenamide hydrochloride 894852-45-0P 894852-90-5P, (E)-N-Methyl-N-[(3-methylbenzofuran-2-yl)methyl]-3-(2-oxo-4-phenyl-2,3,4,5-tetrahydro-1H-pyrido[2,3-e][1,4]diazepin-7-yl)-2-propenamide hydrochloride 894853-53-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(bactericide; compns. comprising multiple antibiotic agents and preparation of heterocycle FabI inhibitor)
RN 709651-33-2 HCAPLUS
CN 2-Propenamide, N-(2-benzofuranylmethyl)-N-methyl-3-(2,3,4,5-tetrahydro-4-methyl-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, monohydrochloride, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

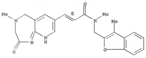
L27 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● HCl

RN 709651-48-9 HCAPLUS
CN 2-Propenamide, N-methyl-N-[(3-methyl-2-benzofuranyl)methyl]-3-(2,3,4,5-tetrahydro-4-methyl-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, monohydrochloride, (2E)- (9CI) (CA INDEX NAME)

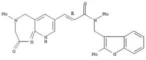
Double bond geometry as shown.



● HCl

RN 709651-53-6 HCAPLUS
CN 2-Propenamide, N-methyl-N-[(2-methyl-3-benzofuranyl)methyl]-3-(2,3,4,5-tetrahydro-4-methyl-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, monohydrochloride, (2E)- (9CI) (CA INDEX NAME)

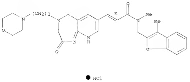
Double bond geometry as shown.



● HCl

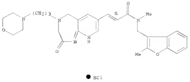
RN 709651-82-1 HCAPLUS
CN 2-Propenamide, N-methyl-N-[(3-methyl-2-benzofuranyl)methyl]-3-[2,3,4,5-tetrahydro-4-[3-(4-morpholinyl)propyl]-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl]-, monohydrochloride, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



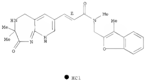
RN 709651-85-4 HCAPLUS
CN 2-Propenamide, N-methyl-N-[(2-methyl-3-benzofuranyl)methyl]-3-[2,3,4,5-tetrahydro-4-[3-(4-morpholinyl)propyl]-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl]-, monohydrochloride, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



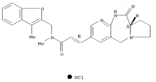
RN 709652-77-7 HCAPLUS
CN 2-Propenamide, N-methyl-N-[(3-methyl-2-benzofuranyl)methyl]-3-(2,3,4,5-tetrahydro-3,3-dimethyl-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, hydrochloride (1:1), (2E)- (CA INDEX NAME)

Double bond geometry as shown.



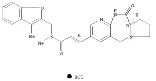
RN 894851-54-8 HCAPLUS
CN 2-Propenamide, 3-[(9aS)-7,8,9,9a,10,11-hexahydro-10-oxo-5H-pyrido[2,3-e]pyrrolo[1,2-a][1,4]diazepin-3-yl]-N-methyl-N-[(3-methyl-2-benzofuranyl)methyl]-, hydrochloride (1:1), (2E)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



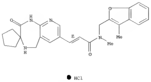
RN 894851-55-9 HCAPLUS
CN 2-Propenamide, 3-[(9aR)-7,8,9,9a,10,11-hexahydro-10-oxo-5H-pyrido[2,3-e]pyrrolo[1,2-a][1,4]diazepin-3-yl]-N-methyl-N-[(3-methyl-2-benzofuranyl)methyl]-, hydrochloride (1:1), (2E)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).
Double bond geometry as shown



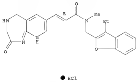
RN 894851-73-1 HCAPLUS
CN 2-Propenamide, N-methyl-N-[(3-methyl-2-benzofuranyl)methyl]-3-(1',2',4',5'-tetrahydro-2'-oxospiro[cyclopentane-1,3'-[3H]pyrido[2,3-e][1,4]diazepin]-7'-yl)-, hydrochloride (1:1), (2E)- (CA INDEX NAME)

Double bond geometry as shown.



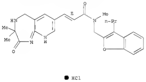
RN 894851-80-0 HCAPLUS
CN 2-Propenamide, N-[(3-ethyl-2-benzofuranyl)methyl]-N-methyl-3-(2,3,4,5-tetrahydro-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, hydrochloride (1:1), (2E)- (CA INDEX NAME)

Double bond geometry as shown.



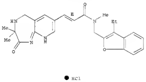
RN 894851-84-4 HCAPLUS
CN 2-Propenamide, N-methyl-N-[(3-propyl-2-benzofuranyl)methyl]-3-(2,3,4,5-tetrahydro-3,3-dimethyl-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, hydrochloride (1:1), (2E)- (CA INDEX NAME)

Double bond geometry as shown.



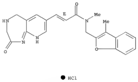
RN 894851-90-2 HCAPLUS
CN 2-Propenamide, N-[(3-ethyl-2-benzofuranyl)methyl]-N-methyl-3-(2,3,4,5-tetrahydro-3,3-dimethyl-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, hydrochloride (1:1), (2E)- (CA INDEX NAME)

Double bond geometry as shown.



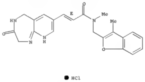
RN 894851-97-9 HCAPLUS
CN 2-Propenamide, N-methyl-N-[(3-methyl-2-benzofuranyl)methyl]-3-(2,3,4,5-tetrahydro-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, hydrochloride (1:1), (2E)- (CA INDEX NAME)

Double bond geometry as shown.



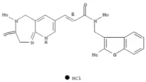
RN 894852-25-6 HCAPLUS
CN 2-Propenamide, N-methyl-N-[(3-methyl-2-benzofuranyl)methyl]-3-(2,3,4,5-tetrahydro-3-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, hydrochloride (1:1), (2E)- (CA INDEX NAME)

Double bond geometry as shown.



RN 894852-32-5 HCAPLUS
CN 2-Propenamide, N-methyl-N-[(2-methyl-3-benzofuranyl)methyl]-3-(2,3,4,5-tetrahydro-4-methyl-3-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, hydrochloride (1:1), (2E)- (CA INDEX NAME)

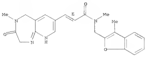
Double bond geometry as shown.



RN 894852-35-8 HCAPLUS
CN 2-Propenamide, N-methyl-N-[(3-methyl-2-benzofuranyl)methyl]-3-(2,3,4,5-tetrahydro-4-methyl-3-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, hydrochloride (1:1), (2E)- (CA INDEX NAME)

Double bond geometry as shown.

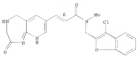
L27 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● HCl

RN 894852-45-0 HCAPLUS
CN 2-Propenamide, N-[(3-chloro-2-benzofuranyl)methyl]-N-methyl-3-(2,3,4,5-tetrahydro-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, monohydrochloride, (2E)- (9CI) (CA INDEX NAME)

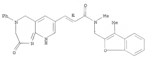
Double bond geometry as shown.



● HCl

RN 894852-90-5 HCAPLUS
CN 2-Propenamide, N-methyl-N-[(3-methyl-2-benzofuranyl)methyl]-3-(2,3,4,5-tetrahydro-2-oxo-4-phenyl-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, hydrochloride (1:1), (2E)- (CA INDEX NAME)

Double bond geometry as shown.



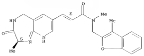
● HCl

RN 894853-53-3 HCAPLUS
CN 2-Propenamide, N-methyl-N-[(3-methyl-2-benzofuranyl)methyl]-3-[(2S)-2,3,4,5-tetrahydro-2-methyl-3-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl]-, (2E)-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

L27 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CRN 894853-52-2
CMF C23 H24 N4 O3

Absolute stereochemistry.
Double bond geometry as shown.

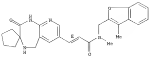


CM 2

CRN 76-05-1
CMF C2 H F3 O2

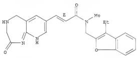
IT 894851-76-4P 894851-82-2P, (E)-N-[(3-Ethylbenzofuran-2-yl)methyl]-N-methyl-3-(2-oxo-2,3,4,5-tetrahydro-1H-pyrido[2,3-e][1,4]diazepin-7-yl)-2-propenamide 894851-89-9P, (E)-3-(3,3-Dimethyl-2-oxo-2,3,4,5-tetrahydro-1H-pyrido[2,3-e][1,4]diazepin-7-yl)-N-methyl-N-[(3-propylbenzofuran-2-yl)methyl]-2-propenamide 894851-92-4P, (E)-3-(3,3-Dimethyl-2-oxo-2,3,4,5-tetrahydro-1H-pyrido[2,3-e][1,4]diazepin-7-yl)-N-[(3-ethylbenzofuran-2-yl)methyl]-N-methyl-2-propenamide 894851-99-1P, (E)-N-Methyl-N-[(3-methylbenzofuran-2-yl)methyl]-3-(2-oxo-2,3,4,5-tetrahydro-1H-pyrido[2,3-e][1,4]diazepin-7-yl)-2-propenamide
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation), RACT (Reactant or reagent)
(intermediate; compns. comprising multiple antibiotic agents and preparation of heterocycle FabI inhibitor)
RN 894851-76-4 HCAPLUS
CN 2-Propenamide, N-methyl-N-[(3-methyl-2-benzofuranyl)methyl]-3-(1',2',4',5'-tetrahydro-2'-oxospiro[cyclopentane-1,3'-[3H]pyrido[2,3-e][1,4]diazepin]-7'-yl)-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



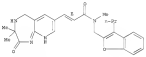
RN 894851-82-2 HCAPLUS
CN 2-Propenamide, N-[(3-ethyl-2-benzofuranyl)methyl]-N-methyl-3-(2,3,4,5-tetrahydro-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, (2E)- (CA INDEX NAME)

L27 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
Double bond geometry as shown.



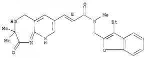
RN 894851-89-9 HCAPLUS
CN 2-Propenamide, N-methyl-N-[(3-propyl-2-benzofuranyl)methyl]-3-(2,3,4,5-tetrahydro-3,3-dimethyl-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



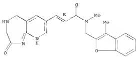
RN 894851-92-4 HCAPLUS
CN 2-Propenamide, N-[(3-ethyl-2-benzofuranyl)methyl]-N-methyl-3-(2,3,4,5-tetrahydro-3,3-dimethyl-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



RN 894851-99-1 HCAPLUS
CN 2-Propenamide, N-methyl-N-[(3-methyl-2-benzofuranyl)methyl]-3-(2,3,4,5-tetrahydro-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



L27 ANSWER 4 OF 5 HCAPLUS COPYRIGHT 2007 ACS on STN
AN 2004:799437 HCAPLUS
DN 141:314353
TI Compositions comprising multiple antibiotic agents including a FabI inhibitor, methods of using the same, and preparation of the heterocycle FabI inhibitors
IN Berman, Judd M.; Schmid, Molly B.; Mendlein, John D.; Kaplan, Nachum
PA Affinium Pharmaceuticals, Inc., Can.
SO PCT Int. Appl., 311 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO2004082586	A2	20040930	2004WO-IB01261	20040317
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	JP2006523207	T	20061012	2006JP-0506526	20040317
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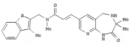
	2003US-476970P	P	20030609		
	2003US-488379P	P	20030718		
	2004WO-IB01261	W	20040317		

OS MARPAT 141:314353
GI



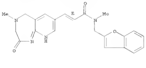
I

AB The invention is directed to antibacterial compns. comprising an NADH (or NADPH)-dependent enoyl-acyl carrier protein (ACP) reductase (FabI, previously designated EnvM) inhibitor of formula (Y1)a-A-CH(R1)-NR1CO-L-R2 (I) and at least one other antibiotic/antibacterial agent [L = alkyl, alkenyl, or cycloalkyl which may be substituted by one or more R1; A = (un)substituted bicyclic heteroaryl of 8-12 atoms or a tricyclic ring of 12-16 atoms, containing 1-4 heteroatoms selected from N, S, and O; R1 = cyclo/alkyl, alk/aryl; R2 = heterocyclyl; a = 0-4, Y1 = -(CH2)n-CO-NR4R5; R4 = water solubilizing group; R5 = H, cyclo/alkyl, n = 0-4]. The antibacterial composition exhibits a synergistic antibacterial effect compared to its individual components. Thus, reacting 7-Bromo-3,3-dimethyl-1,3,4,5-tetrahydropyrido[2,3-e][1,4]diazepin-2-one (preparation given) with N-Methyl-N-[(3-methylbenzo[b]thiophen-2-yl)methyl]acrylamide (preparation given), followed by acidulation gave diazepinone salt II•HCl. Selected I inhibited FabI with a Ki < 1 nM, an MIC (minimal inhibitory concentration) < 0.125 µg/mL, and an IC50 < 10 nM.
IT 709651-33-2P, (E)-N-[(Benzofuran-2-yl)methyl]-N-methyl-3-(4-methyl-2-oxo-2,3,4,5-tetrahydro-1H-pyrido[2,3-e][1,4]diazepin-7-yl)-2-propenamide monohydrochloride 709651-48-9P, (E)-N-Methyl-N-(3-methylbenzofuran-2-ylmethyl)-3-(4-methyl-2-oxo-2,3,4,5-tetrahydro-1H-pyrido[2,3-e][1,4]diazepin-7-yl)-2-propenamide monohydrochloride

L27 ANSWER 4 OF 5 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
709651-53-6P, (E)-N-Methyl-N-(2-methylbenzofuran-3-ylmethyl)-3-(4-methyl-2-oxo-2,3,4,5-tetrahydro-1H-pyrido[2,3-e][1,4]diazepin-7-yl)-2-propenamide monohydrochloride 709651-82-1P, (E)-N-Methyl-N-(3-methylbenzofuran-2-ylmethyl)-3-[4-[3-(morpholin-4-yl)propyl]-2-oxo-2,3,4,5-tetrahydro-1H-pyrido[2,3-e][1,4]diazepin-7-yl]-2-propenamide monohydrochloride 709651-85-4P, (E)-N-Methyl-N-(2-methylbenzofuran-3-ylmethyl)-3-[4-[3-(morpholin-4-yl)propyl]-2-oxo-2,3,4,5-tetrahydro-1H-pyrido[2,3-e][1,4]diazepin-7-yl]-2-propenamide monohydrochloride 709652-79-9P, (E)-3-(3,3-Dimethyl-2-oxo-2,3,4,5-tetrahydro-1H-pyrido[2,3-e][1,4]diazepin-7-yl)-N-methyl-N-[(3-methylbenzofuran-2-yl)methyl]-2-propenamide
RL: PAC (Pharmacological activity), SPN (Synthetic preparation), THU (Therapeutic use), BIOL (Biological study), PREP (Preparation), USES (Uses)
(bactericide; compns. comprising multiple antibiotic agents and prepn. of heterocycle FabI inhibitor)

RN 709651-33-2 HCAPLUS
CN 2-Propenamide, N-(2-benzofuranylmethyl)-N-methyl-3-(2,3,4,5-tetrahydro-4-methyl-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, monohydrochloride, (2E)- (9CI) (CA INDEX NAME)

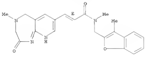
Double bond geometry as shown.



● HCl

RN 709651-48-9 HCAPLUS
CN 2-Propenamide, N-methyl-N-[(3-methyl-2-benzofuranyl)methyl]-3-(2,3,4,5-tetrahydro-4-methyl-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, monohydrochloride, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

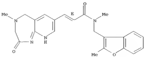


● HCl

RN 709651-53-6 HCAPLUS
CN 2-Propenamide, N-methyl-N-[(2-methyl-3-benzofuranyl)methyl]-3-(2,3,4,5-tetrahydro-4-methyl-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, monohydrochloride, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

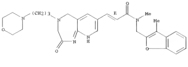
L27 ANSWER 4 OF 5 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● HCl

RN 709651-82-1 HCAPLUS
CN 2-Propenamide, N-methyl-N-[(3-methyl-2-benzofuranyl)methyl]-3-[2,3,4,5-tetrahydro-4-[3-(4-morpholinyl)propyl]-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl]-, monohydrochloride, (2E)- (9CI) (CA INDEX NAME)

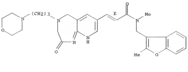
Double bond geometry as shown.



● HCl

RN 709651-85-4 HCAPLUS
CN 2-Propenamide, N-methyl-N-[(2-methyl-3-benzofuranyl)methyl]-3-[2,3,4,5-tetrahydro-4-[3-(4-morpholinyl)propyl]-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl]-, monohydrochloride, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

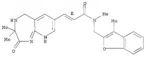


● HCl

RN 709652-79-9 HCAPLUS
CN 2-Propenamide, N-methyl-N-[(3-methyl-2-benzofuranyl)methyl]-3-(2,3,4,5-tetrahydro-3,3-dimethyl-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.

L27 ANSWER 4 OF 5 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L27 ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2007 ACS on STN
AN 2004:515512 HCAPLUS
DN 141:71572
TI Preparation of heterocyclic compounds as antibacterial agents
IN Berman, Judd; Sampson, Peter; Pauls, Heinz W.; Ramnauth, Jailall, Manning, David Douglas; Surman, Matthew David; Xie, Dejian, Decornez, Helene Yvonne
PA Affinium Pharmaceuticals, Inc., Can.
SO PCT Int. Appl., 223 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO2004052890	A1	20040624	2003WO-US38706	20031205
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	RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
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	EP---1575951	A1	20050921	2003EP-0796699	20031205
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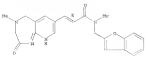
PRAI	2002US-431406P	P	20021206		
	2003US-465583P	P	20030425		
	2003WO-US38706	W	20031205		

OS MARPAT 141:71572
AB Compds. of formula (Y1)a-A-CH(R1)-NR1CO-L-R2 [I; L = a bond, is alkyl, alkenyl, or cycloalkyl which may be substituted with one or more R1; A = a bicyclic heteroaryl ring of 8-12 atoms or a tricyclic ring oft 12-16 atoms, wherein the heteroaryl rings contain 1-4 heteroatoms selected from N, S, and O, and wherein the heteroaryl rings are optionally substituted with one or more groups selected from C1-4 alkyl, CH2OH, OR, SR, CN, N(R)2, CH2N(R)2, NO2, CF3, CO2R, CON(R)2, COR, NRC(O)R, F, Cl, Br, iodo, and S(O)rCF3 (R = H, alkyl, alkaryl; r = 0-2); R1 = H, alkyl, cycloalkyl, aryl, or alkaryl; R2 = heterocyclyl] or pharmaceutically acceptable salts thereof are prepared. These compds. inhibit an NADH (or NADPH)-dependent enoyl-acyl carrier protein (ACP) reductase (FabI, previously designated EnvM) which is believed to be a major biosynthetic enzyme and is a key regulatory point in the overall synthetic pathway of bacterial fatty acid biosynthesis and catalyzes the final step of fatty acid biosynthesis in some bacteria. The present invention also relates to inhibitors and compns. comprising inhibitors of enzymes similar to FabI either structurally or functionally, such as, for example, FabK which is also believed to play a role in bacterial fatty acid synthesis. In another aspect of the present invention, the antibacterial compds. of the present invention may be used to disinfect an inanimate surface by administering the antibacterial compound to the inanimate surface. Thus, (E)-3-(4-methyl-2-oxo-2,3,4,5-tetrahydro-1H-pyrido[2,3-e][1,4]diazepin-7-yl)acrylic acid hydrochloride was condensed with N-methyl-N-(1-propylnaphthalen-2-ylmethyl)amine in DMF using diisopropylethylamine, 1-hydroxybenzotriazole hydrate, and 1-(3-dimethylaminopropyl)-3-ethylcarbodiimide hydrochloride at room temperature for 18 h to give, after silica gel chromatog., 41% (E)-N-Methyl-3-(4-methyl-2-oxo-2,3,4,5-tetrahydro-1H-pyrido[2,3-e][1,4]diazepin-7-yl)-N-[(1-propylnaphthalen-2-yl)methyl]acrylamide as a glassy orange solid and as a mixture of amide rotamers. The compds. I inhibit FabI with a Ki of about 5 pM or less.
IT 709651-33-2P 709651-48-9P 709651-53-6P
709651-82-1P 709651-85-4P 709652-77-7P
709652-79-9P
RL: PAC (Pharmacological activity), SPN (Synthetic preparation), THU (Therapeutic use), BIOL (Biological study), PREP (Preparation), USES (Uses)
(preparation of heterocyclic compds. as enoyl-acyl carrier protein reductase FabI inhibitors and antibacterial agents)
RN 709651-33-2 HCAPLUS

L3? ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 2-Propenamide, N-[2-benzofuranylmethyl]-N-methyl-3-(2,3,4,5-tetrahydro-4-methyl-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, monohydrochloride, (3E)- (9CI) (CA INDEX NAME)

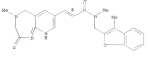
Double bond geometry as shown.



● HCl

RN 709451-19-9 HCAPLUS
CN 2-Propenamide, N-methyl-N-[(3-methyl-2-benzofuranyl)methyl]-3-(2,3,4,5-tetrahydro-4-methyl-5-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, monohydrochloride, (2E)- (9CI) (CA INDEX NAME)

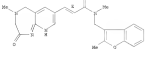
Double bond geometry as shown.



● HCl

RN 709451-53-6 HCAPLUS
CN 2-Propenamide, N-ethyl-N-[(3-methyl-2-benzofuranyl)methyl]-3-(2,3,4,5-tetrahydro-4-methyl-5-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, monohydrochloride, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

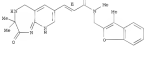


● HCl

RN 709451-83-1 HCAPLUS
CN 2-Propenamide, N-methyl-N-[(3-methyl-2-benzofuranyl)methyl]-3-[2,3,4,5-

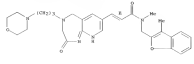
L27 ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(CA INDEX NAME)

Double bond geometry as shown.



L27 ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
tetrahydro-4-[3-(4-morpholinyl)propyl]-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, monohydrochloride, (2E)- (9CI) (CA INDEX NAME)

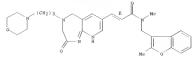
Double bond geometry as shown.



● HCl

RN 709451-85-4 HCAPLUS
CN 2-Propenamide, N-methyl-N-[(2-methyl-3-benzofuranyl)methyl]-3-[2,3,4,5-tetrahydro-4-[3-(4-morpholinyl)propyl]-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl]-, monohydrochloride, (2E)- (9CI) (CA INDEX NAME)

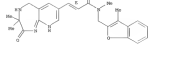
Double bond geometry as shown.



● HCl

RN 709452-77-7 HCAPLUS
CN 2-Propenamide, N-methyl-N-[(5-methyl-2-benzofuranyl)methyl]-3-(2,3,4,5-tetrahydro-3,3-dimethyl-5-oxo-1H-pyrido[2,3-e]-1,4-diazepin-9-yl)-, hydrochloride (1:1), (2E)- (CA INDEX NAME)

Double bond geometry as shown.



● HCl

RN 709452-78-8 HCAPLUS
CN 2-Propenamide, N-methyl-N-[(3-methyl-5-benzofuranyl)methyl]-3-(2,3,4,5-tetrahydro-3,3-dimethyl-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, (2E)-

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-> b uspatall
FILE 'USPATFULL' ENTERED AT 16:37:09 ON 28 NOV 2007
CA INDEXING COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

FILE 'USPATOLD' ENTERED AT 16:37:09 ON 28 NOV 2007
CA INDEXING COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

FILE 'USPAT2' ENTERED AT 16:37:09 ON 28 NOV 2007
CA INDEXING COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

-> d bib abs hitstr 129 tot
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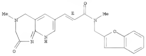
L29 ANSWER 1 OF 2 USPATFULL on STN
AN 2006:215750 USPATFULL
TI Heterocyclic compounds, methods of making them and their use in therapy
IN Berman, Judd, Toronto, CANADA
Sampson, Peter, Ontario, CANADA
Pauls, Heinz W., Ontario, CANADA
Ramnauth, Jailall, Ontario, CANADA
Douglas, David, Manning, NY, UNITED STATES
Surman, Matthew David, Albany, NY, UNITED STATES
Xie, Dejian, Glenmount, NY, UNITED STATES
Decornez, Helene Yvonne, Clifton Park, NY, UNITED STATES
PA Affinium Pharmaceuticals, Inc., Toronto, ON, CANADA, M5J1V6 (non-U.S. corporation)
PI US-20060183908 A1 20060817
AI 2003US-000537747 A1 20031205 (10)
2003WO-US0038706 20031205
20060327 PCT 371 date
PRAI 2002US-000431406P 20021206 (60)
2003US-000465583P 20030425 (60)
DT Utility
FS APPLICATION
LREP FOLEY HOAG, LLP, PATENT GROUP, WORLD TRADE CENTER WEST, 155 SEAPORT BLVD, BOSTON, MA, 02110, US
CLMN Number of Claims: 49
ECL Exemplary Claim: 1
DRWN 8 Drawing Page(s)
LN.CNT 7935
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB In part, the present invention is directed to antibacterial compounds of formula (I) wherein A is a bicyclic heteroaryl ring or a tricyclic ring and R.sub.2 is an heterocyclic residue; L is a bond, or L is alkyl, alkenyl or cycloalkyl ##STR1##

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT 709651-33-2P 709651-48-9P 709651-53-6P
709651-82-1P 709651-85-4P 709652-77-7P
709652-79-9P
(preparation of heterocyclic compds. as enoyl-acyl carrier protein reductase FabI inhibitors and antibacterial agents)
RN 709651-33-2 USPATFULL
CN 2-Propenamide, N-(2-benzofuranylmethyl)-N-methyl-3-(2,3,4,5-tetrahydro-4-methyl-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, monohydrochloride, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

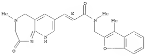


● HCl

RN 709651-48-9 USPATFULL
CN 2-Propenamide, N-methyl-N-[(3-methyl-2-benzofuranyl)methyl]-3-(2,3,4,5-tetrahydro-4-methyl-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, monohydrochloride, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

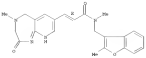
L29 ANSWER 1 OF 2 USPATFULL on STN (Continued)



● HCl

RN 709651-53-6 USPATFULL
CN 2-Propenamide, N-methyl-N-[(2-methyl-3-benzofuranyl)methyl]-3-(2,3,4,5-tetrahydro-4-methyl-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, monohydrochloride, (2E)- (9CI) (CA INDEX NAME)

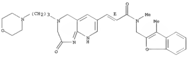
Double bond geometry as shown.



● HCl

RN 709651-82-1 USPATFULL
CN 2-Propenamide, N-methyl-N-[(3-methyl-2-benzofuranyl)methyl]-3-[2,3,4,5-tetrahydro-4-[3-(4-morpholinyl)propyl]-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl]-, monohydrochloride, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

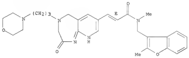


● HCl

RN 709651-85-4 USPATFULL
CN 2-Propenamide, N-methyl-N-[(2-methyl-3-benzofuranyl)methyl]-3-[2,3,4,5-tetrahydro-4-[3-(4-morpholinyl)propyl]-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl]-, monohydrochloride, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

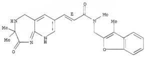
L29 ANSWER 1 OF 2 USPATFULL on STN (Continued)



● HCl

RN 709652-77-7 USPATFULL
CN 2-Propenamide, N-methyl-N-[(3-methyl-2-benzofuranyl)methyl]-3-(2,3,4,5-tetrahydro-3,3-dimethyl-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, hydrochloride (1:1), (2E)- (CA INDEX NAME)

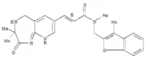
Double bond geometry as shown.



● HCl

RN 709652-79-9 USPATFULL
CN 2-Propenamide, N-methyl-N-[(3-methyl-2-benzofuranyl)methyl]-3-(2,3,4,5-tetrahydro-3,3-dimethyl-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, (2E)- (CA INDEX NAME)

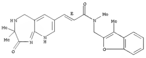
Double bond geometry as shown.



L29 ANSWER 2 OF 2 USPATFULL on STN
AN 2006:167754 USPATFULL
TI Compositions comprising multiple bioactive agents, and methods of using the same
IN Berman, Judd M., Toronto, CANADA
Schmid, Molly B., Toronto, CANADA
Mendlein, John D., Encinitas, CA, UNITED STATES
Kaplan, Nachum, Toronto, CANADA
PA Affinium Pharmaceuticals, Inc., Toronto, CANADA (non-U.S. corporation)
PI US-20060142265 A1 20060629
AI 2005US-000231298 A1 20050919 (11)
RLI Continuation-in-part of Ser. No. 2004WO-IB0001261, filed on 17 Mar 2004, UNKNOWN
PRAI 2003US-000455189P 20030317 (60)
2003US-000476970P 20030609 (60)
2003US-000488379P 20030718 (60)
DT Utility
FS APPLICATION
LREP FOLEY HOAG, LLP, PATENT GROUP, WORLD TRADE CENTER WEST, 155 SEAPORT BLVD, BOSTON, MA, 02110, US
CLMN Number of Claims: 42
ECL Exemplary Claim: 1
DRWN 10 Drawing Page(s)
LN.CNT 15944
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB In part, the present invention is directed to compositions comprising a FabI inhibitor and at least one other bioactive agent. In another part, the present invention is directed to antibacterial compositions comprising a compound of formulas I-III and at least one other antibacterial agent.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT 709652-79-9P, (E)-3-(3,3-Dimethyl-2-oxo-2,3,4,5-tetrahydro-1H-pyrido[2,3-e][1,4]diazepin-7-yl)-N-methyl-N-[(3-methylbenzofuran-2-yl)methyl]-2-propenamide
(bactericide; compns. comprising multiple antibiotic agents and preparation of heterocycle FabI inhibitor)
RN 709652-79-9 USPATFULL
CN 2-Propenamide, N-methyl-N-[(3-methyl-2-benzofuranyl)methyl]-3-(2,3,4,5-tetrahydro-3,3-dimethyl-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.

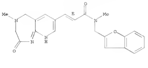


IT 709651-33-2P, (E)-N-[(Benzofuran-2-yl)methyl]-N-methyl-3-(4-methyl-2-oxo-2,3,4,5-tetrahydro-1H-pyrido[2,3-e][1,4]diazepin-7-yl)-2-propenamide monohydrochloride 709651-48-9P, (E)-N-Methyl-N-(3-methylbenzofuran-2-ylmethyl)-3-(4-methyl-2-oxo-2,3,4,5-tetrahydro-1H-pyrido[2,3-e][1,4]diazepin-7-yl)-2-propenamide monohydrochloride 709651-53-6P, (E)-N-Methyl-N-(2-methylbenzofuran-3-ylmethyl)-3-(4-methyl-2-oxo-2,3,4,5-tetrahydro-1H-pyrido[2,3-e][1,4]diazepin-7-yl)-2-propenamide monohydrochloride 709651-82-1P, (E)-N-Methyl-N-(3-methylbenzofuran-2-ylmethyl)-3-[4-[3-(morpholin-4-yl)propyl]-2-oxo-2,3,4,5-tetrahydro-1H-pyrido[2,3-e][1,4]diazepin-7-yl]-2-propenamide monohydrochloride 709651-85-4P, (E)-N-Methyl-N-(2-methylbenzofuran-3-ylmethyl)-3-[4-[3-(morpholin-4-yl)propyl]-2-oxo-2,3,4,5-tetrahydro-1H-pyrido[2,3-e][1,4]diazepin-7-yl]-2-propenamide monohydrochloride 709652-77-7P 894851-54-8P 894851-55-9P 894851-73-1P 894851-80-0P, (E)-N-[(3-Ethylbenzofuran-2-yl)methyl]-N-methyl-3-(2-oxo-2,3,4,5-tetrahydro-1H-pyrido[2,3-e][1,4]diazepin-7-yl)-2-propenamide hydrochloride 894851-84-4P 894851-90-2P 894851-97-9P, (E)-N-Methyl-N-[(3-

L29 ANSWER 2 OF 2 USPATFULL on STN (Continued)
methylbenzofuran-2-yl)methyl]-3-(2-oxo-2,3,4,5-tetrahydro-1H-pyrido[2,3-e][1,4]diazepin-7-yl)-2-propenamide hydrochloride 894852-25-6P, (E)-N-Methyl-N-[(3-methylbenzofuran-2-yl)methyl]-3-(3-oxo-2,3,4,5-tetrahydro-1H-pyrido[2,3-e][1,4]diazepin-7-yl)-2-propenamide hydrochloride 894852-32-5P, (E)-N-Methyl-N-[(2-methylbenzofuran-3-yl)methyl]-3-(4-methyl-3-oxo-2,3,4,5-tetrahydro-1H-pyrido[2,3-e][1,4]diazepin-7-yl)-2-propenamide hydrochloride 894852-35-8P, (E)-N-Methyl-N-[(3-methylbenzofuran-2-yl)methyl]-3-(4-methyl-3-oxo-2,3,4,5-tetrahydro-1H-pyrido[2,3-e][1,4]diazepin-7-yl)-2-propenamide hydrochloride 894852-45-0P 894852-90-5P, (E)-N-Methyl-N-[(3-methylbenzofuran-2-yl)methyl]-3-(2-oxo-4-phenyl-2,3,4,5-tetrahydro-1H-pyrido[2,3-e][1,4]diazepin-7-yl)-2-propenamide hydrochloride 894853-53-3P
(bactericide; compns. comprising multiple antibiotic agents and prepn. of heterocycle FabI inhibitor)

RN 709651-33-2 USPATFULL
CN 2-Propenamide, N-(2-benzofuranylmethyl)-N-methyl-3-(2,3,4,5-tetrahydro-4-methyl-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, monohydrochloride, (2E)- (9CI) (CA INDEX NAME)

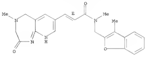
Double bond geometry as shown.



● HCl

RN 709651-48-9 USPATFULL
CN 2-Propenamide, N-methyl-N-[(3-methyl-2-benzofuranyl)methyl]-3-(2,3,4,5-tetrahydro-4-methyl-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, monohydrochloride, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

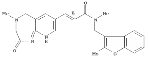


● HCl

RN 709651-53-6 USPATFULL
CN 2-Propenamide, N-methyl-N-[(2-methyl-3-benzofuranyl)methyl]-3-(2,3,4,5-tetrahydro-4-methyl-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, monohydrochloride, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

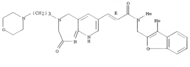
L29 ANSWER 2 OF 2 USPATFULL on STN (Continued)



● HCl

RN 709651-82-1 USPATFULL
CN 2-Propenamide, N-methyl-N-[(3-methyl-2-benzofuranyl)methyl]-3-[2,3,4,5-tetrahydro-4-[3-(4-morpholinyl)propyl]-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl]-, monohydrochloride, (2E)- (9CI) (CA INDEX NAME)

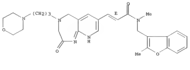
Double bond geometry as shown



● HCl

RN 709651-85-4 USPATFULL
CN 2-Propenamide, N-methyl-N-[(2-methyl-3-benzofuranyl)methyl]-3-[2,3,4,5-tetrahydro-4-[3-(4-morpholinyl)propyl]-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl]-, monohydrochloride, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

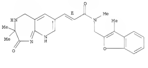


● HCl

RN 709652-77-7 USPATFULL
CN 2-Propenamide, N-methyl-N-[(3-methyl-2-benzofuranyl)methyl]-3-(2,3,4,5-tetrahydro-3,3-dimethyl-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, hydrochloride (1:1), (2E)- (CA INDEX NAME)

Double bond geometry as shown.

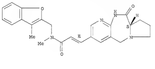
L29 ANSWER 2 OF 2 USPATFULL on STN (Continued)



● HCl

RN 894851-54-8 USPATFULL
CN 2-Propenamide, 3-[(9aS)-7,8,9,9a,10,11-hexahydro-10-oxo-5H-pyrido[2,3-e]pyrrolo[1,2-a][1,4]diazepin-3-yl]-N-methyl-N-[(3-methyl-2-benzofuranyl)methyl]-, hydrochloride (1.1), (2E)- (CA INDEX NAME)

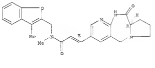
Absolute stereochemistry. Rotation (+).
Double bond geometry as shown.



● HCl

RN 894851-55-9 USPATFULL
CN 2-Propenamide, 3-[(9aR)-7,8,9,9a,10,11-hexahydro-10-oxo-5H-pyrido[2,3-e]pyrrolo[1,2-a][1,4]diazepin-3-yl]-N-methyl-N-[(3-methyl-2-benzofuranyl)methyl]-, hydrochloride (1:1), (2E)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).
Double bond geometry as shown.

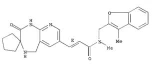


● HCl

RN 894851-73-1 USPATFULL
CN 2-Propenamide, N-methyl-N-[(3-methyl-2-benzofuranyl)methyl]-3-(1',2',4',5'-tetrahydro-2'-oxospiro[cyclopentane-1,3'-[3H]pyrido[2,3-e][1,4]diazepin]-7'-yl)-, hydrochloride (1:1), (2E)- (CA INDEX NAME)

Double bond geometry as shown.

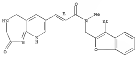
L29 ANSWER 2 OF 2 USPATFULL on STN (Continued)



● HCl

RN 894851-80-0 USPATFULL
CN 2-Propenamide, N-[(3-ethyl-2-benzofuranyl)methyl]-N-methyl-3-(2,3,4,5-tetrahydro-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, hydrochloride (1:1), (2E)- (CA INDEX NAME)

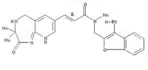
Double bond geometry as shown.



● HCl

RN 894851-84-4 USPATFULL
CN 2-Propenamide, N-methyl-N-[(3-propyl-2-benzofuranyl)methyl]-3-(2,3,4,5-tetrahydro-3,3-dimethyl-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, hydrochloride (1.1), (2E)- (CA INDEX NAME)

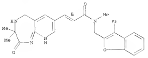
Double bond geometry as shown.



● HCl

RN 894851-90-2 USPATFULL
CN 2-Propenamide, N-[(3-ethyl-2-benzofuranyl)methyl]-N-methyl-3-(2,3,4,5-tetrahydro-3,3-dimethyl-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, hydrochloride (1:1), (2E)- (CA INDEX NAME)

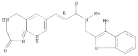
Double bond geometry as shown.



● HCl

RN 894851-97-9 USPATFULL
CN 2-Propenamide, N-methyl-N-[(3-methyl-2-benzofuranyl)methyl]-3-(2,3,4,5-tetrahydro-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, hydrochloride (1:1), (2E)- (CA INDEX NAME)

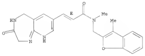
Double bond geometry as shown



● HCl

RN 894852-25-6 USPATFULL
CN 2-Propenamide, N-methyl-N-[(3-methyl-2-benzofuranyl)methyl]-3-(2,3,4,5-tetrahydro-3-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, hydrochloride (1:1), (2E)- (CA INDEX NAME)

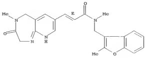
Double bond geometry as shown



● HCl

RN 894852-32-5 USPATFULL
CN 2-Propenamide, N-methyl-N-[(2-methyl-3-benzofuranyl)methyl]-3-(2,3,4,5-tetrahydro-4-methyl-3-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, hydrochloride (1:1), (2E)- (CA INDEX NAME)

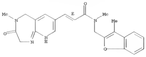
Double bond geometry as shown.



● HCl

RN 894852-35-8 USPATFULL
CN 2-Propenamide, N-methyl-N-[(3-methyl-2-benzofuranyl)methyl]-3-(2,3,4,5-tetrahydro-4-methyl-3-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, hydrochloride (1:1), (2E)- (CA INDEX NAME)

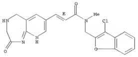
Double bond geometry as shown.



● HCl

RN 894852-45-0 USPATFULL
CN 2-Propenamide, N-[(3-chloro-2-benzofuranyl)methyl]-N-methyl-3-(2,3,4,5-tetrahydro-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, monohydrochloride, (2E)- (9CI) (CA INDEX NAME)

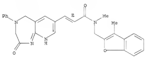
Double bond geometry as shown.



● HCl

RN 894852-90-5 USPATFULL
CN 2-Propenamide, N-methyl-N-[(3-methyl-2-benzofuranyl)methyl]-3-(2,3,4,5-tetrahydro-2-oxo-4-phenyl-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, hydrochloride (1:1), (2E)- (CA INDEX NAME)

Double bond geometry as shown.



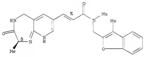
● HCl

RN 894853-53-3 USPATFULL
CN 2-Propenamide, N-methyl-N-[(3-methyl-2-benzofuranyl)methyl]-3-[(2S)-2,3,4,5-tetrahydro-2-methyl-3-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl]-, (2E)-, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 894853-52-2
CMF C23 H24 N4 O3

Absolute stereochemistry.
Double bond geometry as shown.

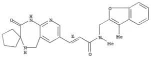


CM 2

CRN 76-05-1
CMF C2 H F3 O2

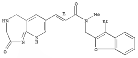
IT 894851-76-4P 894851-82-2P, (E)-N-[(3-Ethylbenzofuran-2-yl)methyl]-N-methyl-3-(2-oxo-2,3,4,5-tetrahydro-1H-pyrido[2,3-e][1,4]diazepin-7-yl)-2-propenamide 894851-89-9P, (E)-3-(3,3-Dimethyl-2-oxo-2,3,4,5-tetrahydro-1H-pyrido[2,3-e][1,4]diazepin-7-yl)-N-methyl-N-[(3-propylbenzofuran-2-yl)methyl]-2-propenamide 894851-92-4P, (E)-3-(3,3-Dimethyl-2-oxo-2,3,4,5-tetrahydro-1H-pyrido[2,3-e][1,4]diazepin-7-yl)-N-[(3-ethylbenzofuran-2-yl)methyl]-N-methyl-2-propenamide 894851-99-1P, (E)-N-Methyl-N-[(3-methylbenzofuran-2-yl)methyl]-3-(2-oxo-2,3,4,5-tetrahydro-1H-pyrido[2,3-e][1,4]diazepin-7-yl)-2-propenamide
(intermediate, compns. comprising multiple antibiotic agents and preparation of heterocycle FabI inhibitor)
RN 894851-76-4 USPATFULL
CN 2-Propenamide, N-methyl-N-[(3-methyl-2-benzofuranyl)methyl]-3-(1',2',4',5'-tetrahydro-2'-oxospiro[cyclopentane-1,3'-[3H]pyrido[2,3-e][1,4]diazepin]-7'-yl]-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



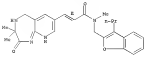
RN 894851-82-2 USPATFULL
CN 2-Propenamide, N-[(3-ethyl-2-benzofuranyl)methyl]-N-methyl-3-(2,3,4,5-tetrahydro-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



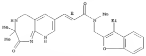
RN 894851-89-9 USPATFULL
CN 2-Propenamide, N-methyl-N-[(3-propyl-2-benzofuranyl)methyl]-3-(2,3,4,5-tetrahydro-3,3-dimethyl-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.



RN 894851-92-4 USPATFULL
CN 2-Propenamide, N-[(3-ethyl-2-benzofuranyl)methyl]-N-methyl-3-(2,3,4,5-tetrahydro-3,3-dimethyl-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, (2E)- (CA INDEX NAME)

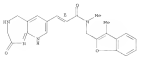
Double bond geometry as shown.



RN 894851-99-1 USPATFULL
CN 2-Propenamide, N-methyl-N-[(3-methyl-2-benzofuranyl)methyl]-3-(2,3,4,5-tetrahydro-2-oxo-1H-pyrido[2,3-e]-1,4-diazepin-7-yl)-, (2E)- (CA INDEX NAME)

L19 ANSWER 3 OF 3 USPATFULL on STN (Continued)

Double bond geometry as shown.



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-> d his

     (FILE 'HOME' ENTERED AT 15:53:37 ON 28 NOV 2007)

     FILE 'HCAPLUS' ENTERED AT 15:53:47 ON 28 NOV 2007
L1             1 US20060183908/PN

     FILE 'REGISTRY' ENTERED AT 15:53:52 ON 28 NOV 2007

     FILE 'HCAPLUS' ENTERED AT 15:53:52 ON 28 NOV 2007
L2             TRA L1 1- RN :      478 TERMS

     FILE 'REGISTRY' ENTERED AT 15:53:52 ON 28 NOV 2007
L3           478 SEA L2
L4            18 L3 AND OC4-C6/ES
L5             7 L4 AND NC5-NC2NC3/ES
L6            39 C24H26N4O3 AND OC4-C6/ES
L7             3 L6 AND NC5-NC2NC3/ES
                 SEL RN 2-3
L8             2 E1-2 AND L7

     FILE 'HCAPLUS' ENTERED AT 16:03:24 ON 28 NOV 2007
L9             4 L8

     FILE 'REGISTRY' ENTERED AT 16:16:06 ON 28 NOV 2007
L10            5 L5 NOT L8

     FILE 'HCAPLUS' ENTERED AT 16:16:24 ON 28 NOV 2007
L11            3 L10

     FILE 'REGISTRY' ENTERED AT 16:17:11 ON 28 NOV 2007
L12              STR
L13           39 L12
L14         4856 L12 FULL
                 SAV TEM J747C1/A L14
L15           35 L14 AND NC5-NC2NC3/ES
L16            7 L15 AND L3

     FILE 'HCAPLUS' ENTERED AT 16:24:39 ON 28 NOV 2007
L17            5 L15
L18            4 L17 AND L9,L11
L19            1 L17 NOT L18

     FILE 'REGISTRY' ENTERED AT 16:27:30 ON 28 NOV 2007
L20          316 L14 AND NRRS>=3
L21              STR L12
L22            3 L21 SAM SUB=L14
L23           42 L21 FULL SUB=L14
                 SAV TEM L23 J747C1N/A

     FILE 'HCAPLUS' ENTERED AT 16:31:53 ON 28 NOV 2007
L24            5 L23
L25            4 L24 AND L9,L11
L26            1 L24 NOT L25
L27            5 L9,L11,L17-19,L24-26

     FILE 'HCAOLD' ENTERED AT 16:33:45 ON 28 NOV 2007
L28            0 L23

     FILE 'USPATFULL, USPATOLD, USPAT2' ENTERED AT 16:34:42 ON 28 NOV 2007
L29            2 L23

     FILE 'BIOSIS' ENTERED AT 16:35:42 ON 28 NOV 2007
L30            0 L23

     FILE 'EMBASE' ENTERED AT 16:35:54 ON 28 NOV 2007
L31            0 L23

     FILE 'MEDLINE' ENTERED AT 16:36:01 ON 28 NOV 2007
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L32 0 L23

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